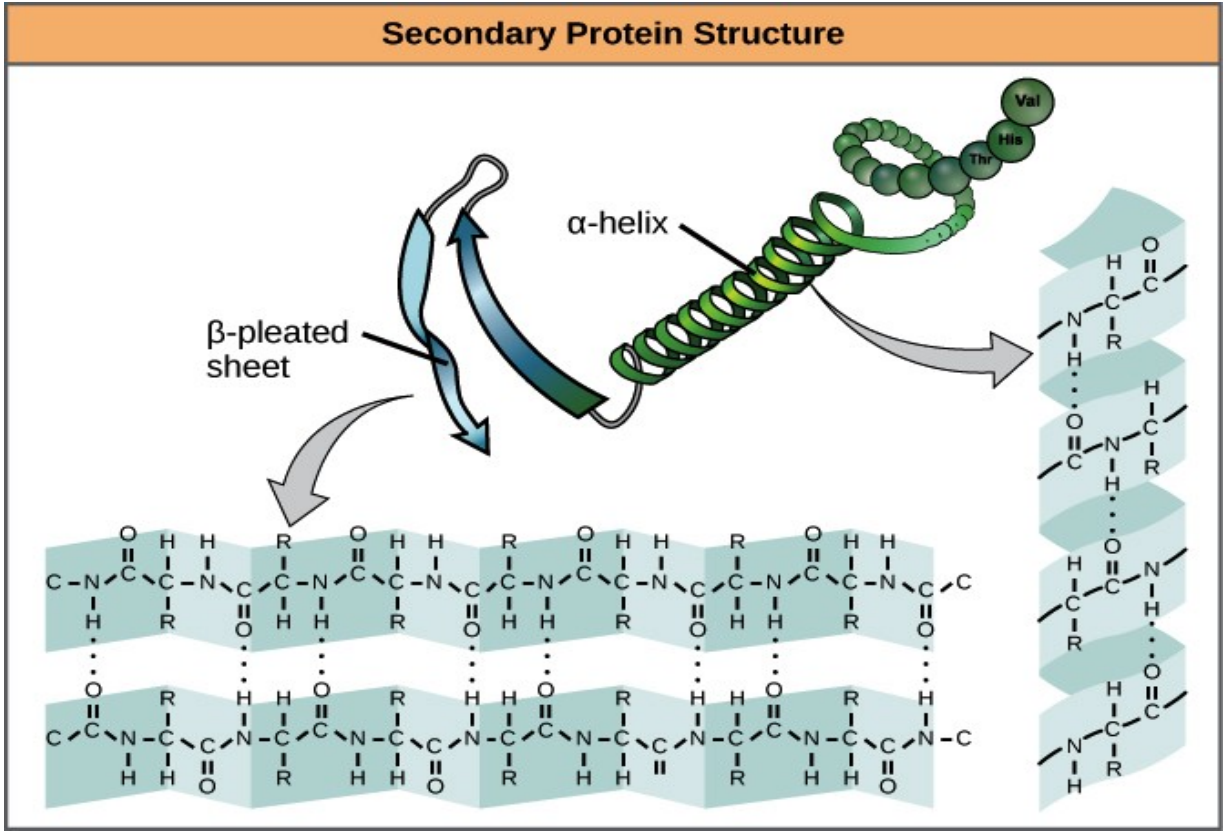
Assignment of protein secondary structure



Summary

1. Secondary protein structure

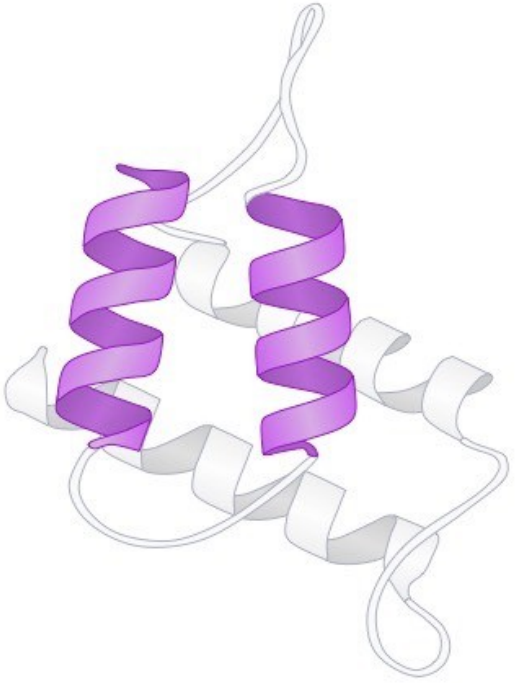
2.DSSP method

3. Data preparation

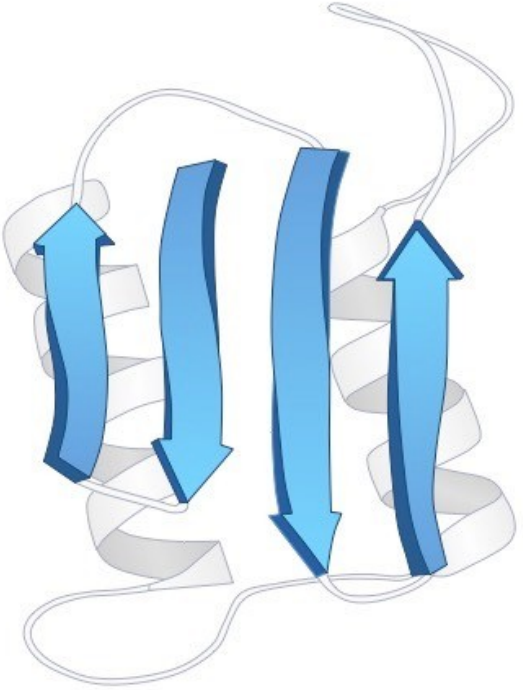
4. Program

5. Results

Secondary Protein Structure



α - helices



β - pleated sheets

DSSP method

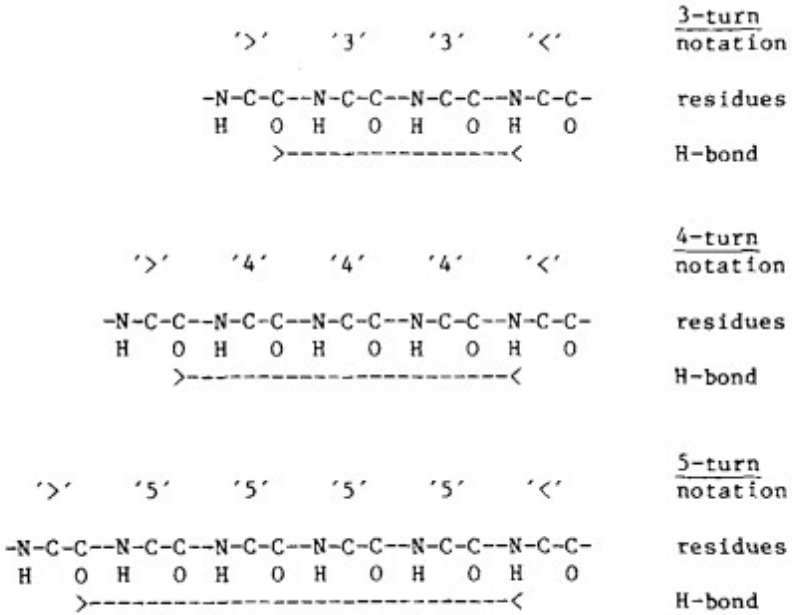
- *DSSP is an algorithm*
- *Secondary structure assignment through H-bonds*
- *No prediction from secondary structure*
- *Output 8 differents secondary structures*

Data preparation

PDB = Protein Data Bank

HBPLUS recognizes H-bond and creates new file

Program : definition of turn and helix



A turn is an H-bond between a residue and a second one located at 3, 4 or 5 residues further down the chain

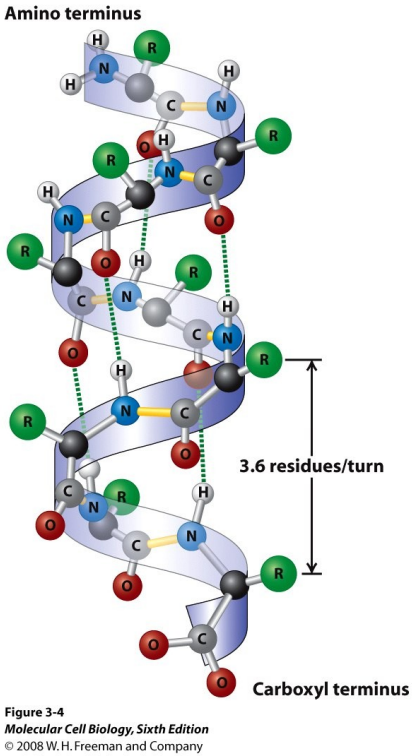
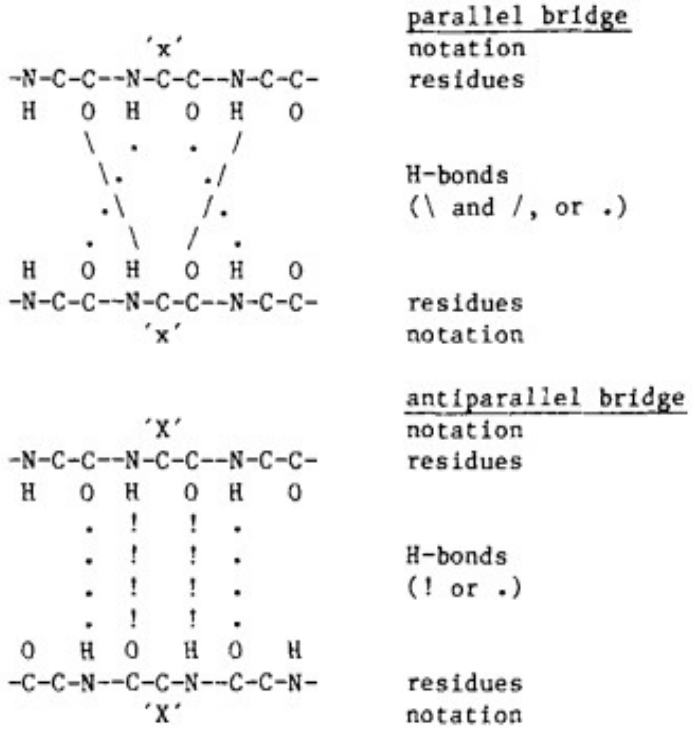


Figure 3-4
Molecular Cell Biology, Sixth Edition

An helix is a succession of N-turn

Program : definition of bridge

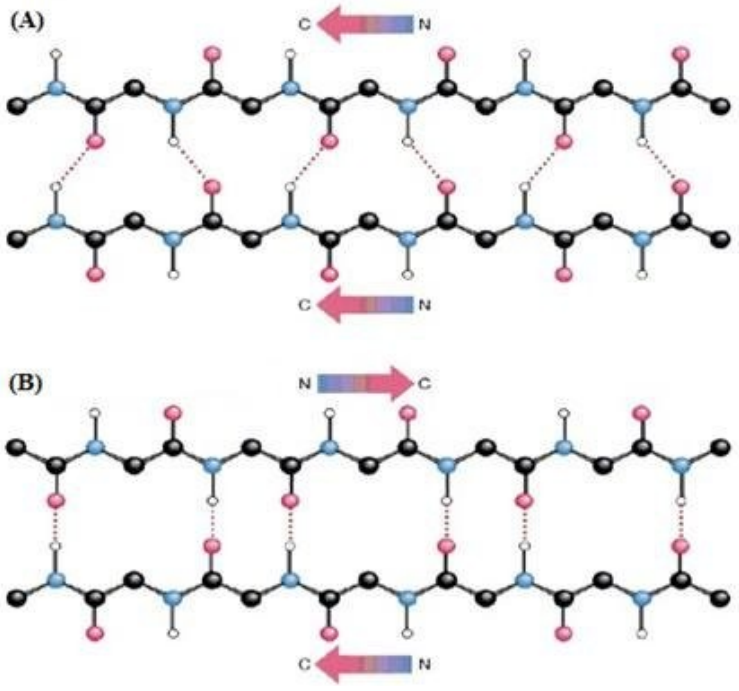


Define a donnor residue (i) and an acceptor residue (j)

Parallel bridge is H-bond (i-1, j) and H-bond (j, i+1), or H-bond (j-1, i) and H-bond (i, j+1)

Anti-parallel bridge is H-bond (i, j) and H-bond (j, i), or H-bond (i-1, j+1) and H-bond (j-1, i+1)

Program : definition of ladder and sheet



A ladder is succession of one or more bridges

A sheet is one or more ladders connected by shared residues

My results

numéro résidu	structure
1	-
2	-
3	ladder
4	ladder
5	ladder
6	-
7	-
8	-
9	-
10	-
11	-
12	-
13	-
14	-
15	-
16	-
17	ladder
18	-
19	ladder
20	-

21	-
22	hélice
23	hélice
24	hélice
25	hélice
26	hélice
27	hélice
28	hélice
29	hélice
30	hélice
31	hélice
32	-
33	-
34	-
35	-
36	-
37	ladder
38	-

39	-
40	hélice
41	hélice
42	hélice
43	hélice
44	hélice
45	hélice
46	hélice
47	hélice
48	hélice
49	hélice
50	hélice
51	-

My program will insign an structure to a residue if it did find one

DSSP results

#	RESIDUE	AA	STRUCTURE	BP1	BP2
1	1	A	M	0	0
2	2	A	K E +A	20	0A
3	3	A	V E -AB	19	38A
4	4	A	I E -AB	18	37A
5	5	A	F E - B	0	36A
6	6	A	L S S+	0	0
7	7	A	K S S-	0	0
8	8	A	D -	0	0
9	9	A	V B >> -C	13	0B
10	10	A	K T 34 S+	0	0
11	11	A	G T 34 S+	0	0
12	12	A	K T <4 S-	0	0
13	13	A	G B < -C	9	0B
14	14	A	K > -	0	0
15	15	A	K T 3 S+	0	0
16	16	A	G T 3 S+	0	0
17	17	A	E < -	0	0
18	18	A	I E +A	4	0A
19	19	A	K E -A	3	0A
20	20	A	N E +A	2	0A
21	21	A	V -	0	0
22	22	A	A > -	0	0
23	23	A	D H > S+	0	0
24	24	A	G H > S+	0	0
25	25	A	Y H >>S+	0	0
26	26	A	A I <>S+	0	0
27	27	A	N I <5S+	0	0
28	28	A	N I <5S+	0	0
29	29	A	F I X5S+	0	0
30	30	A	L I 4XS+	0	0
31	31	A	F T >4<S+	0	0
32	32	A	K T 345S+	0	0
33	33	A	Q T 3<5S-	0	0
34	34	A	G T < 5S+	0	0
35	35	A	L S <S+	0	0
36	36	A	A E -B	5	0A
37	37	A	I E -B	4	0A
38	38	A	E E -B	3	0A
39	39	A	A +	0	0
40	40	A	T > -	0	0
41	41	A	P H > S+	0	0
42	42	A	A H > S+	0	0
43	43	A	N H > S+	0	0
44	44	A	L H X S+	0	0
45	45	A	K H X S+	0	0
46	46	A	A H X S+	0	0
47	47	A	L H X S+	0	0
48	48	A	E H < S+	0	0
49	49	A	A H < S+	0	0
50	50	A	Q H <	0	0
51	51	A	K <	0	0

You can compare my output with DSSP output

Thank you for your attention